WHAT IS CLAIMED IS:

1. A process for identifying compounds as potential ligands for a protein having a ligand-binding site, comprising:

a) determining secondary structural elements of the protein that constitute the ligand-binding site;

b) breaking down the molecular surface of the ligand-biding site of the protein into molecular surface elements;

(c) identifying known molecular surface patches that are complementary to a neighboring molecular surface element;

(d) effecting coordinate transformation of the molecular surface patches identified in step c) with a neighboring molecular surface element, based on a starting element at an rms value less than 2Å;

(e) identifying counterparts of the molecular surface patches in known compounds; and

(f) assessing the fit of the compounds identified in step (e) in terms of local packing density, wherein a better fit indicates a better potential for the compounds to be ligands of the protein.

2. The process as described in claim 1, wherein external surfaces of the secondary structures of the ligand binding site are determined in step (b).

3. The process as described in claim 1 wherein the known molecular surface patches are superposed with the secondary structural elements.

4. The process as described in Claim 1 wherein the molecular surface patches lie on atoms of the binding site after a coordinate transformation.

5. The process as described in Claim 1, wherein the identified ligands are compared with a known initial protein plus ligand.

6. The process as described in claim 1, wherein the ligands are peptides.

7. The process as described in claim 1 wherein the proteins are enzymes.

8. The process as described in claim 1, wherein the rms value is 1.5 Å.

9. The process of Claim 1 wherein the known molecular surface patches are identified from a database.

10. The process of Claim 1 wherein the known neighboring element is a receptor or an enzyme.

11. The process as described in claim 6, wherein the peptides comprise at least 10 amino acids.

12. The process as described in claim 6 wherein the peptides are subsequently transformed into a peptidomimetic.

13. A process of determining the structure of a protein, comprising: identifying ligands from known molecular surface patches using the process of claim 1; and determining the structure of the protein based on the known structure of the neighboring element to which the molecular surface patches bind.

14. The process as described in claim 2, wherein the molecular surface patches create contact with said external surfaces.